COMPUTATIONAL ASPECTS OF CONTINUUM DISLOCATION MECHANICS

A. Acharya and **A. Roy**

Department of Civil & Environmental Engineering
Carnegie Mellon University
Pittsburgh, PA 15213
acharyaamit@cmu.edu
anishr@andrew.cmu.edu

We present a field theory of dislocations for the analysis of mechanical response in small volumes. The theory provides a framework for the rigorous determination of the stress field(s) and temporal evolution of a single, a few, or a distribution of dislocation(s) in a crystal, along with the associated deformations produced due to dislocation motion. The constitutive inputs of the theory are specifications only for crystal elasticity and dislocation velocity and nucleation.

In this presentation, issues that arise in the finite element implementation of the above theory will be discussed. The discussion will be in the context of a small-deformation, isotropic version of the theory. The system of field equations admits wave type solutions for the tensorial dislocation density state variable. The dislocation density field acts as the source for the incompatible part of the elastic distortion field. The compatible part of the elastic distortion is determined from the total displacement gradient field and the plastic distortion field, the latter's evolution being specified by the dislocation flux field. In addition, the equations of equilibrium have to be solved, where the stress tensor depends on the elastic distortion.

The numerical algorithm involves finite element discretization methods for equilibrium problems (Galerkin discretization), first-order wave propagation problems (least-squares finite element strategies), and for a linear differential operator ('curl' in the incompatibility equation) which is neither 'one-to-one' nor 'onto'. The resulting algorithm is novel in the context of solving field equations in solid mechanics and requires careful consideration to ensure existence and uniqueness of discrete numerical solutions. Such issues will be discussed in the talk as well as their algorithmic resolution and results will be presented.